CHLORANTHALACTONE A

66395-02-6 | DTXSID90318686

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (7	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 4.40 days

Global applicability domain: Outside

Local applicability domain index: 2.19e-01

Confidence level: 8.75e-01

Nearest Neighbors from the Training Set

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1-Methyl-2-propylbenzene

Measured: 12.5 Predicted: 3.17

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9-Ethyl-9H-fluorene Measured: 2330 Predicted: N/A

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5-Methylindan Measured: 4.93 Predicted: 2.25

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1H-Indene, 2-methyl-Measured: 12.5 Predicted: 2.48

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3-Ethyltoluene Measured: 12.5 Predicted: 3.26